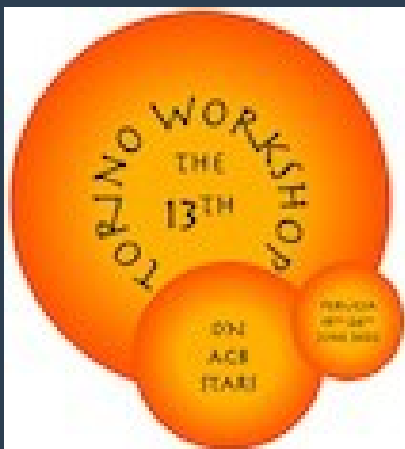


**Mixed Metal Oxides  
as primary dust condensates  
OR  
the “corundum conundrum”**

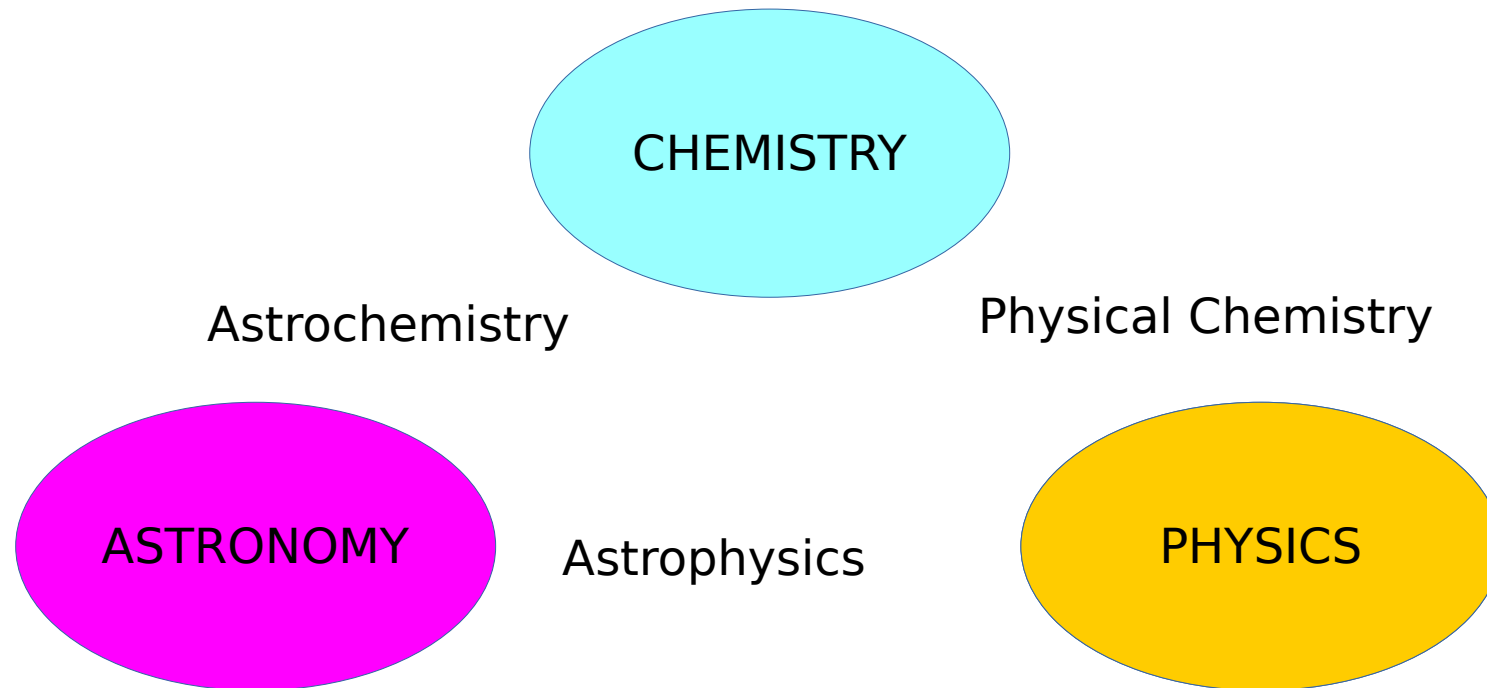


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GOTHENBURG**

# Dust formation: An interdisciplinary study



# Dust formation: An interdisciplinary study

$$|\text{cat}\rangle = \alpha \left| \begin{array}{c} \text{cat} \\ \text{sitting} \end{array} \right\rangle + \beta \left| \begin{array}{c} \text{cat} \\ \text{lying} \end{array} \right\rangle$$

Molecular abundances  
Dust features  
Gas conditions

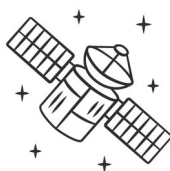
OBSERVATIONS

THEORY

Dust composition:  
Meteoritic stardust  
Analogues of dust  
Reaction rates

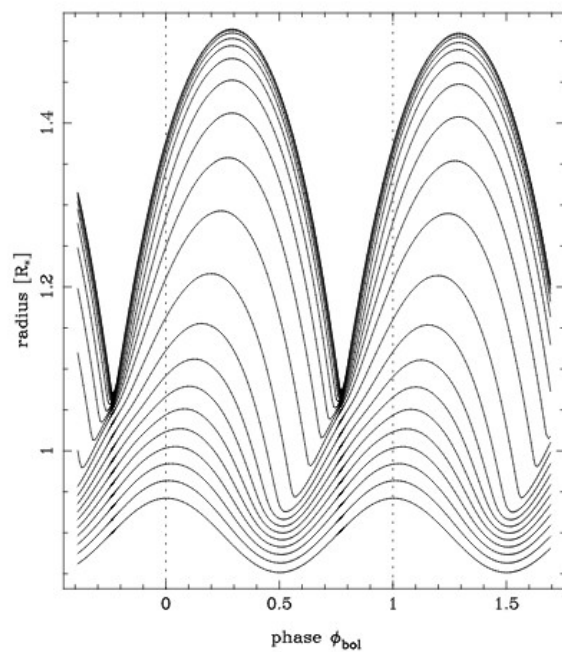
LABORATORY EXPERIMENTS

Spectroscopic constants  
Level transitions

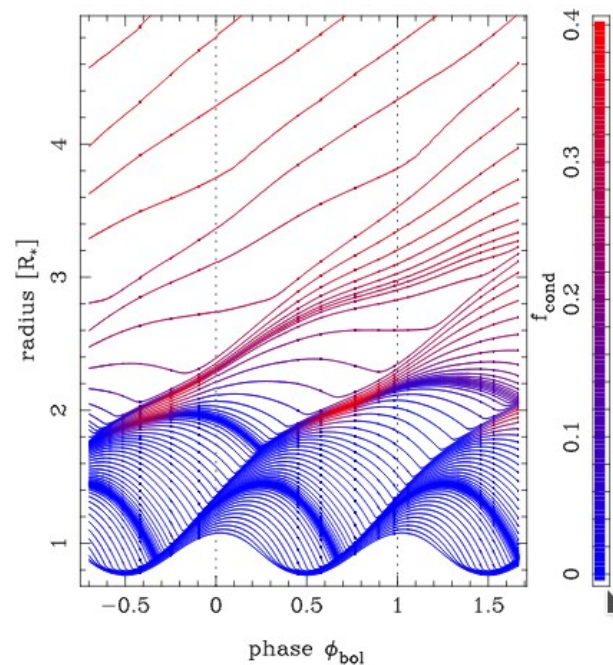


# AGB stars loose mass

- **Stellar mass-loss is a result of stellar pulsations & dust formation**



Without condensates  
Hoefner and coworkers

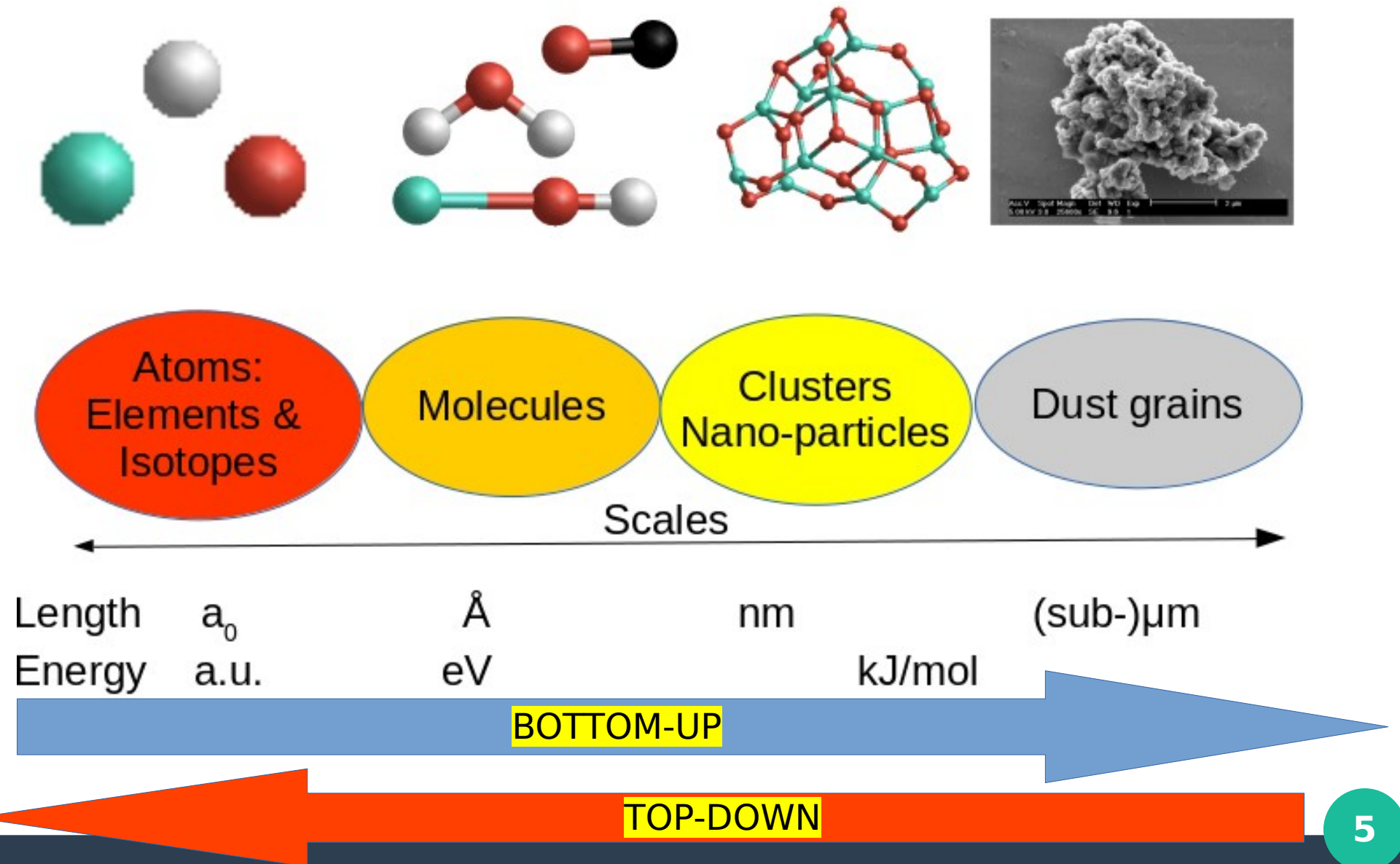


pre-existing dust seeds

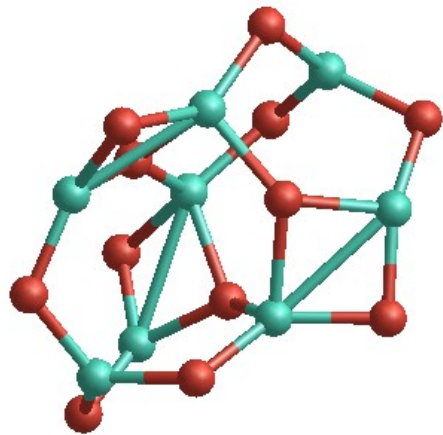
“Pulsations alone cannot drive a mass loss” Woitke (2006)

VULCAN project  
Cristallo et al. 2021

# Nucleation theory: Nano clusters



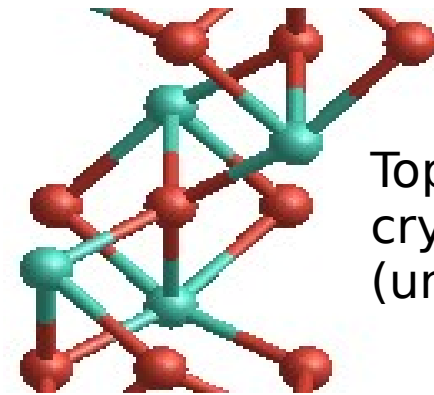
# Bottom-up nucleation



Bottom-up

Most stable  
( $\text{Al}_2\text{O}_3$ )<sub>4</sub>

5 Å  
(0.5 nm)



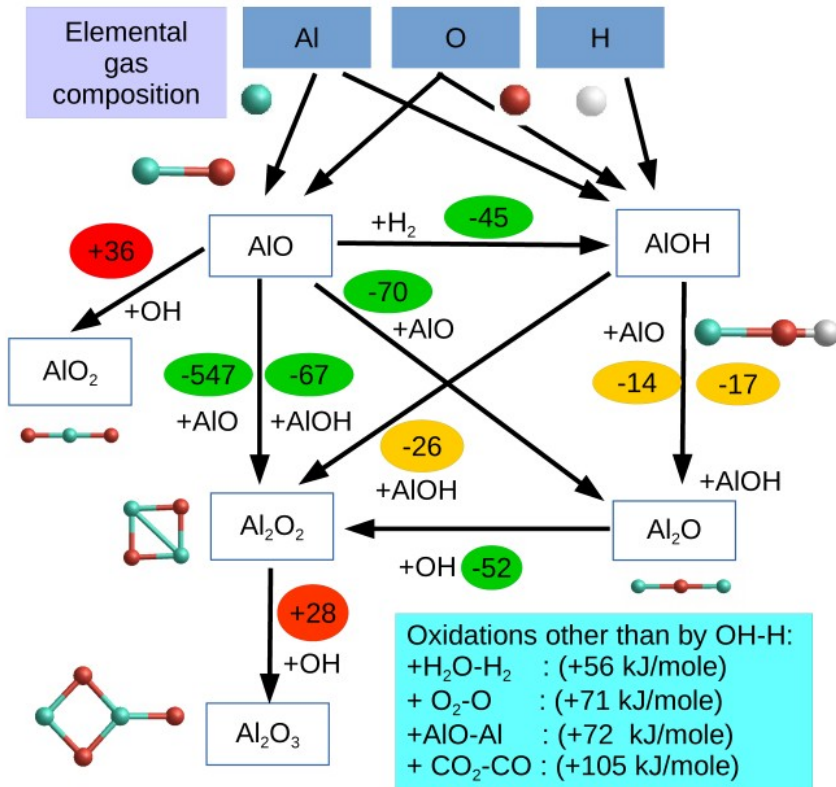
Top-down  
crystal cut  
(unstable)

Clusters: Quantum and finite size effects, different bond characteristics

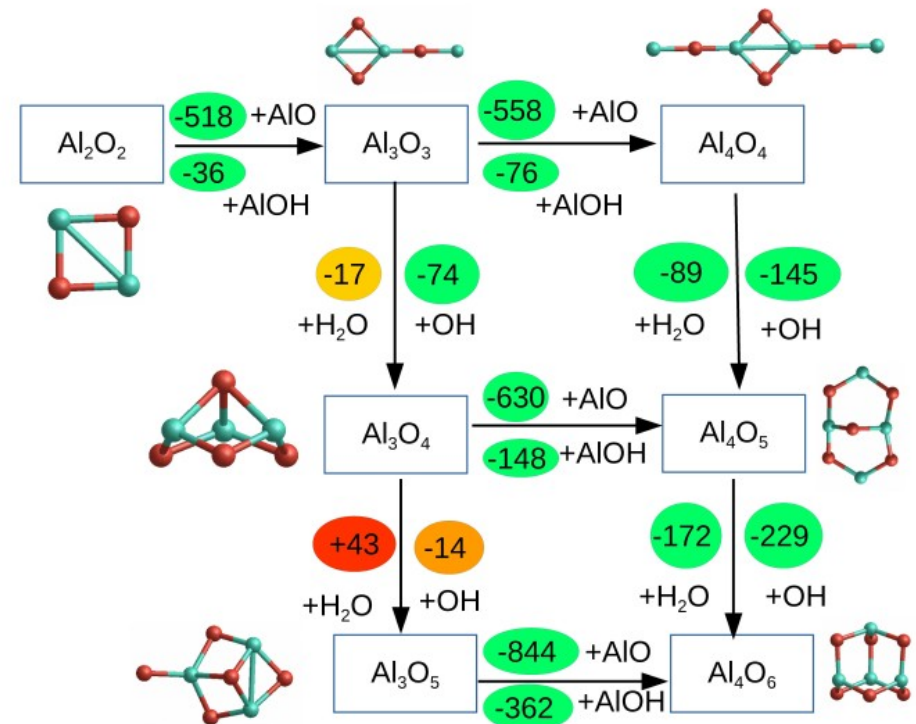
=> potential energies, structures, charges, bonds differ significantly from the crystal (bulk material)

=> Top-down derived clusters **do not represent favourable structures on the (sub-)nano scale**

# Chemical networks: Viability



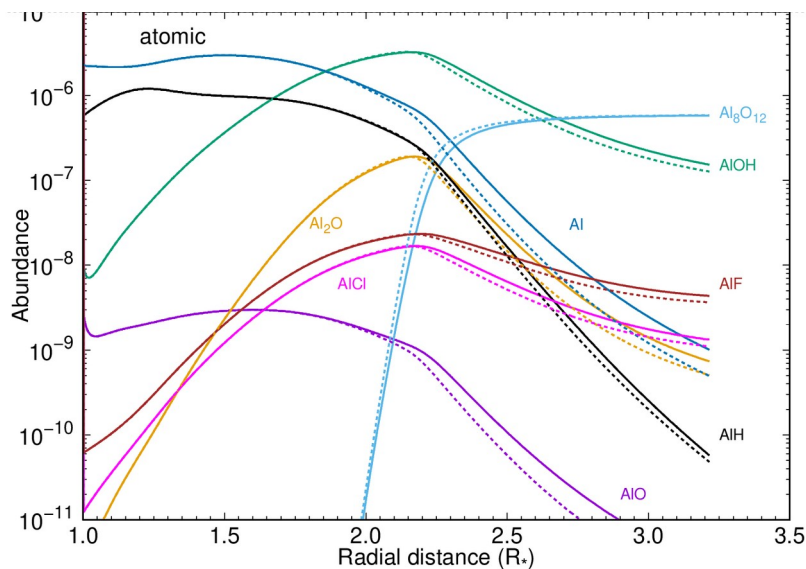
Gobrecht et al 2022



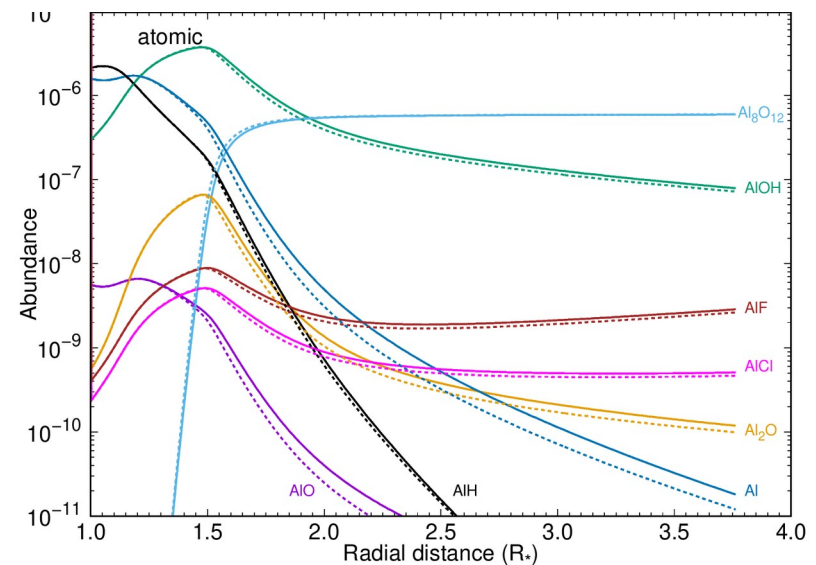
The monomer formation is unfavorable (from atomic gas, AlO and AlOH), but the dimer formation is energetically viable

# Results: Non-pulsating models

Monotonic Outflow describe with  $\beta$ -velocity law



Semi-Regular AGB star (SRV-like)  
 $n_0 = 1. \text{e}14 \text{ cm}^{-3}$ ,  $T_0 = 2400\text{K}$ ,  
 $v_\infty = 5.7 \text{ km/s}$

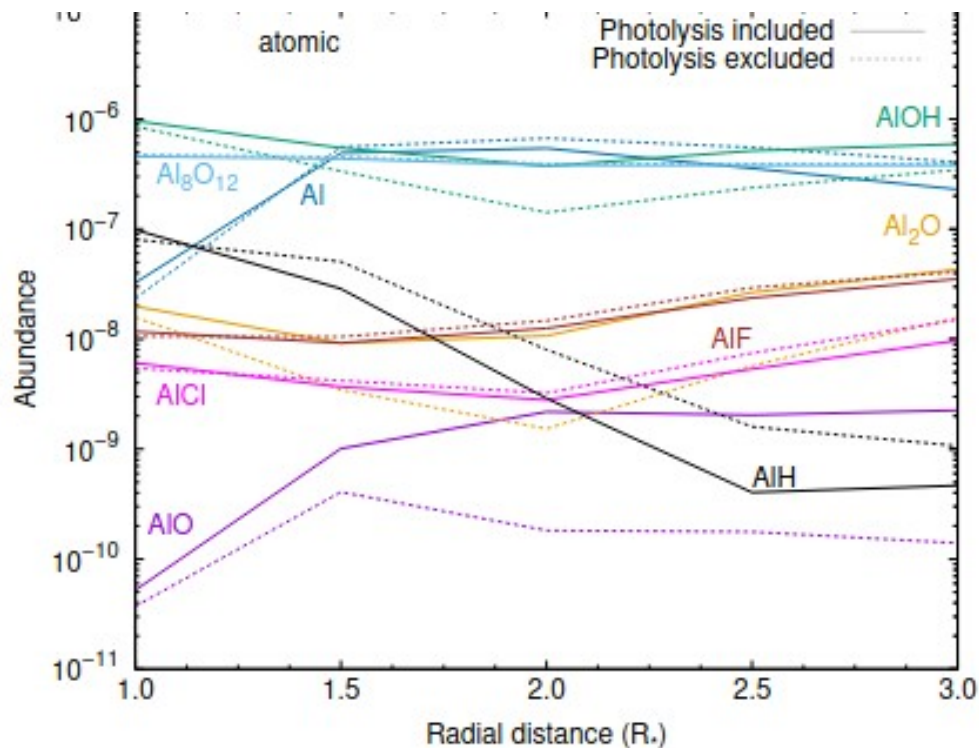


Regular AGB star (Mira-like)  
 $n_0 = 4. \text{e}14 \text{ cm}^{-3}$ ,  $T_0 = 2000\text{K}$ ,  
 $v_\infty = 17.7 \text{ km/s}$

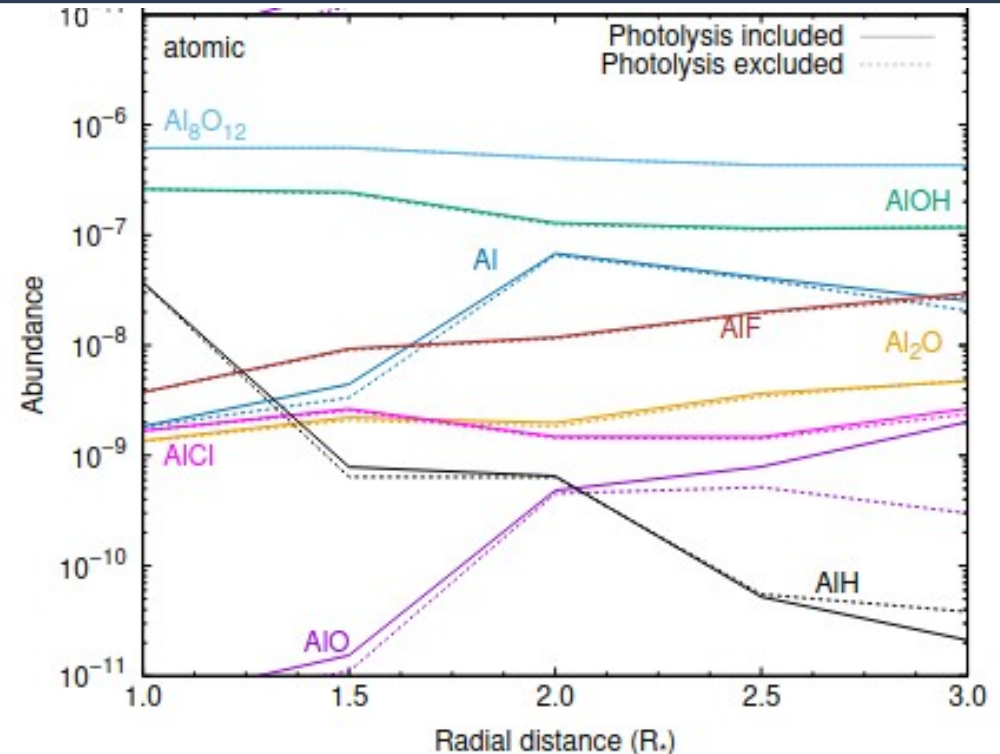
Gobrecht et al 2022



# Results: Pulsating models II



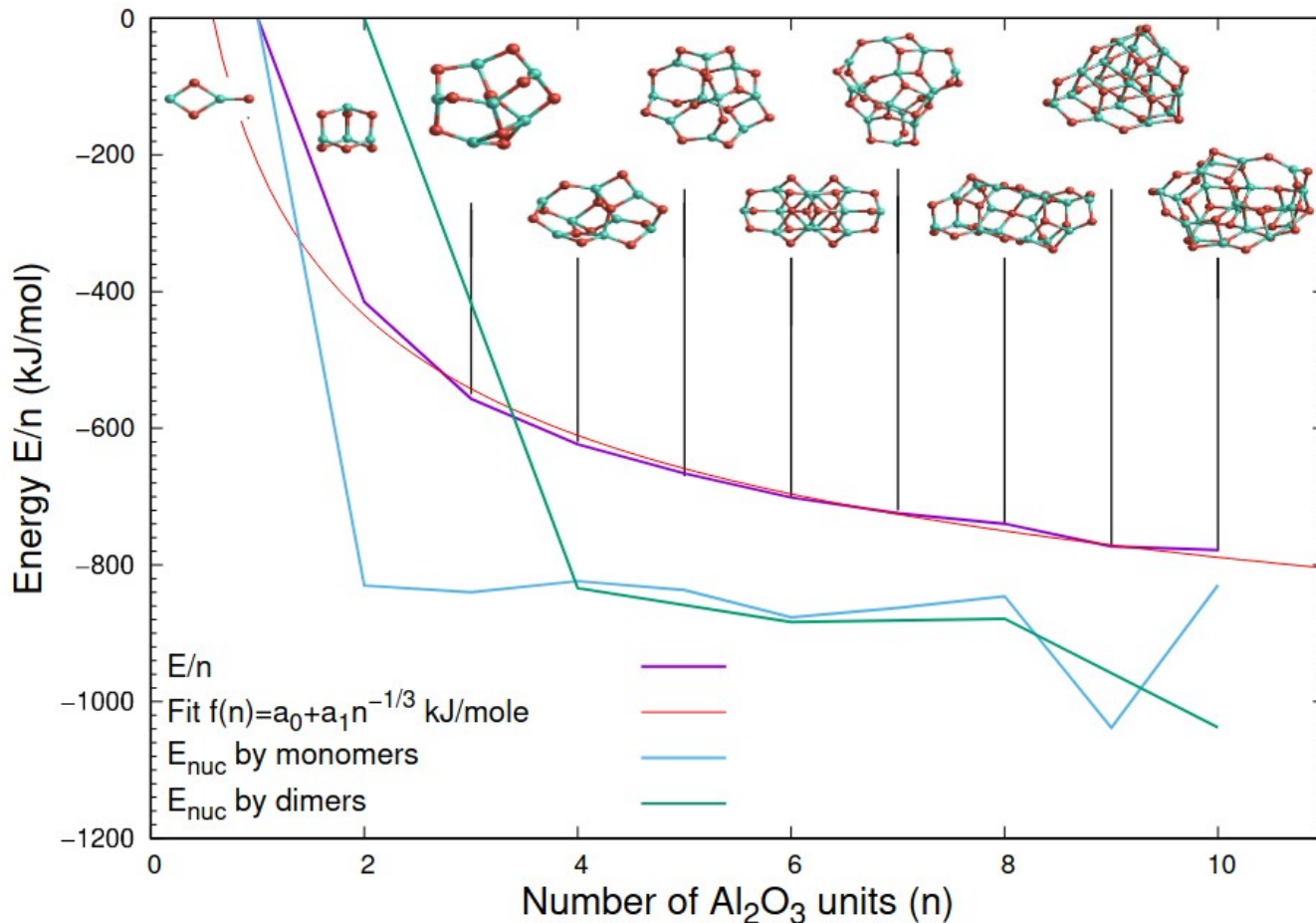
SRV-type AGB star  
( $P=332\text{d}$ ,  $v_s=10\text{ km/s}$ )



MIRA-type AGB star  
( $P=450\text{d}$ ,  $v_s=20\text{ km/s}$ )

Molecule and cluster abundances as a function of **radial distance** after a complete pulsation cycle

# Results: Homogeneous Nucleation



New global minima candidates for  $n=7-10$

Some size more favourable ( $n=3,9$ ), than others ( $n=1,8$ )

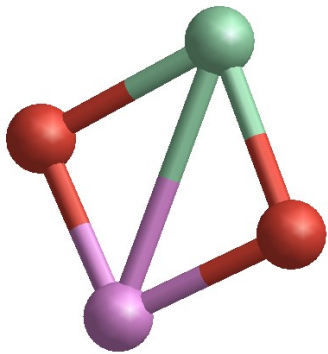
Energy of larger clusters can be approximately extrapolated by a bottom-up fit

Homogeneous nucleation is energetically downhill

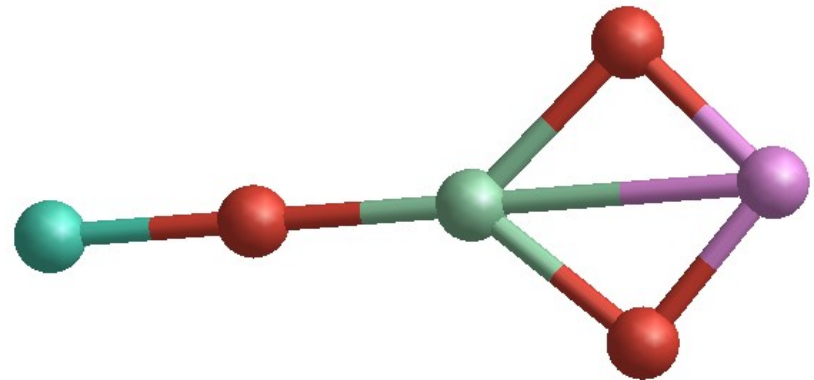
Gobrecht et al 2022

# Mixed metal oxide clusters

- Ternary oxides (i. e. with more than 1 metal) can be even more favourable



**SiTiO<sub>2</sub>**



**AlTiSiO<sub>4</sub>**

# Summary

- **Bottom-up nucleation and chemical-kinetics are key to model dust formation realistically**
- **Homogeneous alumina nucleation is viable proceeding via the dimer ( $n=2$ ) without involving the monomer ( $n=1$ )**
- **Heterogeneous nucleation is a likely alternative in a chemical rich AGB star atmosphere**

**Thanks for your  
attention!**

**Questions?**